

EXHIBIT A

Ethyl acetate

From Wikipedia, the free encyclopedia

Ethyl acetate (systematically, ethyl ethanoate, commonly abbreviated *EA*) is the organic compound with the formula $\text{CH}_3\text{CH}_2\text{OC}(\text{O})\text{CH}_3$. This colorless liquid has a characteristic, not unpleasant smell (similar to pear drops) like certain glues or nail polish removers, in which it is used. As the ester derived from ethanol and acetic acid, thus commonly abbreviated EtOAc, it is manufactured on a large scale for use as a solvent.

Contents

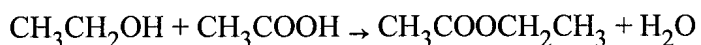
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- 3 Industrial production
- 4 Uses
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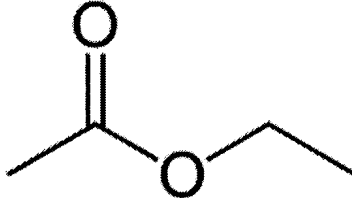
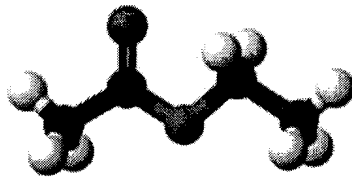
Properties

Ethyl acetate is a moderately polar solvent that has the advantages of being volatile, relatively non-toxic, and non-hygroscopic. It is a weak hydrogen bond acceptor, and is not a donor due to the lack of an acidic proton (one directly bonded to an electronegative atom such as fluorine, oxygen, or nitrogen). Ethyl acetate can dissolve up to 3% water and has a solubility of 8% in water at room temperature. At elevated temperature its solubility in water is higher. It is unstable in the presence of strong aqueous bases and acids.

Preparation

Ethyl acetate is synthesized via the Fischer esterification reaction from acetic acid and ethanol, typically in the presence of an acid catalyst such as sulfuric acid.



Ethyl acetate	
	
	
IUPAC name	Ethyl ethanoate
Other names	ethyl ester, acetic ester, ester of ethanol
Identifiers	
CAS number	[141-78-6]
RTECS number	AH5425000
SMILES	CCOC(C)=O
Properties	
Molecular formula	C ₄ H ₈ O ₂
Molar mass	88.105 g/mol
Appearance	colorless liquid
Density	0.897 g/cm ³ , liquid
Melting point	−83.6 °C (189.55 K)
Boiling point	77.1 °C (350.25 K)
Solubility in water	8.3 g/100 mL (20 °C)
Solubility in ethanol, acetone, diethyl ether, benzene	miscible
MSDS	External MSDS
Main hazards	Flammable (F), Irritant (Xi)
Refractive index	1.3720
CEP A 704	0
Viscosity	0.426 cP at 25 °C
Structure	
Dipole moment	1.78 D

Industrial production

Industrially, ethyl acetate can be produced by the catalytic dehydrogenation of ethanol. For cost reasons, this method is primarily applied to conversion of surplus ethanol feedstock as opposed to predetermined generation on an industrial scale. In addition, it is commonly accepted as far less practical and less cost effective.

Catalysts for dehydrogenation include copper, operating at an elevated temperature but below 250 °C. The copper may have its surface area increased by depositing it on zinc, promoting the growth of snowflake, fractal like, structures. This surface area can be again increased by deposition onto a zeolite, typically ZSM-5. Traces of rare earth metals or alkalies, such as that of sodium and potassium, have also been found to be beneficial to the process. Byproducts of hydrogenation include diethyl ether (thought to primarily arise due to aluminum sites in the catalyst), acetaldehyde, acetaldehyde aldol products, higher esters and ketones. Acetaldehyde and MEK complicate conversion and purification as ethanol forms an azeotrope with water, as does ethyl acetate with ethanol and water and MEK with both ethanol and the acetate. To obtain a high purity product, these azeotropes must be "broken", and this can be achieved by making use of pressure swing distillation.

The composition of the distillate removed from the conversion products is biased towards acetate at atmospheric pressure and ethanol at increased pressure. First, the raw product is fed into a high pressure column where the bulk of the contaminating ethanol is removed. By then feeding the ethanol depleted distillate into a low pressure column, the acetate can be removed from the remaining ethanol azeotrope.


MEK forms during the conversion process from 2-butanol. The latter fails to form an azeotrope with the acetate and so MEK can be removed by hydrogenation of the contaminated product over nickel and further distillation to strip away 2-butanol. This provides the simultaneous benefit of removing the acetylaldehyde contaminant by returning it to an ethanol form and is easily accomplished as hydrogen is a byproduct of the initial dehydrogenation process.

It may also be possible to break the azeotropes with the use of membrane distillation, molecular sieves, an entrainer or absorption medium.

The distilled ethanol and rehydrogenated contaminants can then be recycled into the raw feedstock.

Uses

Solvent

	
R-phrases	R67
S-phrases	S16, S26, S33
Flash point	−4 °C
Related compounds	
Related carboxylate esters	Methyl acetate, Propyl acetate, Butyl acetate
Related compounds	Acetic acid, ethanol
Supplementary data page	
Structure and properties	<i>n</i> , <i>ε</i> _r , etc.
Thermodynamic data	Phase behaviour Solid, liquid, gas
Spectral data	UV, IR, NMR, MS
Except where noted otherwise, data are given for materials in their standard state (at 25 °C, 100 kPa) Infobox disclaimer and references	

Ethyl acetate is primarily used as a solvent. For example, it is commonly used to dissolve the pigments for nail varnishes, and is responsible for the solvent-effect of some nail varnish remover (acetone and acetonitrile are also used). Industrially it is used to decaffeinate coffee beans and tea leaves. It is also used in paints as an activator or hardener.

In the laboratory, a mixture of ethyl acetate and hexane is the most common solvent system used as a chromatography solvent. It is also used as a solvent for extractions. It is rarely used as a reaction mixture because it is prone to hydrolysis.

Like most simple esters, ethyl acetate has a fruity smell. Ethyl acetate is present in confectionery, perfumes, and fruits. In perfumes, it evaporates quickly, leaving but the scent of the perfume on the skin.

Occurrence in wines

Ethyl acetate is present in wines. It may be considered a contaminant at too high concentrations, as typically occurs when wine is exposed to air for a prolonged period. When present at too high concentration in wine, it is regarded as an off-flavor.

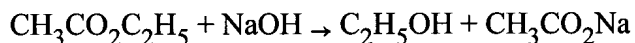
Other uses

In the field of entomology, ethyl acetate is an effective poison for use in insect collecting and study. In a killing jar charged with ethyl acetate, the vapors will kill the collected (usually adult) insect quickly without destroying it. Because it is not hygroscopic, ethyl acetate also keeps the insect soft enough to allow proper mounting suitable for a collection.

Reactions

Ethyl acetate can be hydrolyzed in acid or basic conditions to regain acetic acid and ethanol. The use of an acid catalyst such as sulfuric acid gives poor yields due to it being an equilibrium — the reverse reaction of the Fischer esterification.

To obtain high yields, it is preferable to use a stoichiometric amount of strong base, such as sodium hydroxide. This reaction gives ethanol and sodium acetate, which is not able to react with ethanol any longer:



References

- *Chembytes e-zine - Team effort: Steve Colley describes work to develop a new route to make ethyl acetate starting from low grade renewable feedstocks* (2001)[1]
(http://www.chemsoc.org/chembytes/ezine/2001/colley_aug01.htm#)
- *Ingenia Online - Renewable Processing: The Green Alternative; Using Bio-Ethanol To Manufacture An Industrial Solvent by Mike Ashley* (Issue 29, 2006)[2]
(<http://www.ingenia.org.uk/ingenia/articles.aspx?index=403&print=true>)

External links

- Material safety data (MSDS) (<http://www.jtbaker.com/msds/englishhtml/e2850.htm>) for ethyl acetate
- National Pollutant Inventory - Ethyl acetate fact sheet (<http://www.npi.gov.au/database/substance-info/profiles/38.html>)
- Ethyl Acetate: Molecule of the Month (<http://www.chm.bris.ac.uk/motm/ethylacetate/ethylh.htm>)
- Purpose of Using Concentrated Sulfuric Acid in Esterification for Catalysis (<http://hsc.csu.edu.au/chemistry/core/acidic/chem935/chem935net.html#net4>)
- SEKAB Specification (<http://www.sekab.com/Eng/Informationssidor/Produktblad/Microsoft%20Word%20-%20New%20Ethyl%20acetate.DOC.165.pdf>)
- A Techno Commercial Profile of Ethyl Acetate in India (http://www.chemicalweekly.com/Profiles/Ethyl_Acetate.pdf)

Retrieved from "http://en.wikipedia.org/wiki/Ethyl_acetate"

Categories: Flavors | Acetates | Carboxylate esters | Ester solvents

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EXHIBIT B

Butanone

From Wikipedia, the free encyclopedia

Butanone is a manufactured organic chemical. It is a colorless liquid with a sharp, sweet butterscotch odor reminiscent of acetone. It is a ketone, also known as **methyl ethyl ketone (MEK)**.

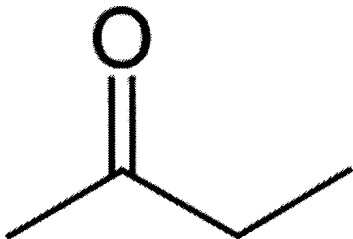
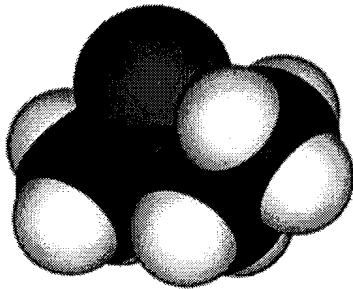
Butanone is produced in large quantities. Nearly half of it is used in paints and other coatings because it will quickly evaporate. It dissolves many substances and is used as a solvent in processes involving gums, resins, cellulose acetate and nitrocellulose coatings and in vinyl films. It is also used in the synthetic rubber industry. It is used in manufacturing plastics, textiles, in the production of paraffin wax, and in household products such as lacquer, varnishes, paint remover, a denaturing agent for denatured alcohol, glues and as a cleaning agent. It is used for synthesis of methyl ethyl ketone peroxide, a catalyst for some polymerization reactions. It is highly flammable. It is not considered a large health threat.

Butanone occurs as a natural product. It is made by some trees and found in some fruits and vegetables in small amounts. It is also released to the air from car and truck exhausts.

Health effects

The known health effects to people from exposure to butanone are slight irritation of the nose, throat, skin, and eyes. There are no known cases of any humans dying from breathing butanone alone. It is basically harmless. However, if butanone is breathed along with other chemicals that damage health, it can increase the amount of damage that occurs.

Serious health effects in animals have been seen only at very high levels. When breathed, these effects included birth defects (Schwetz et al. 1991. Fund. Appl. Toxicol. 16:742-748), loss of consciousness, and death. When swallowed, rats had nervous system effects including drooping eyelids and uncoordinated muscle movements. There was no damage to

Butanone	
	
	
Other names	Methyl ethyl ketone (MEK); Methylpropanone; Ethylmethylketone
Identifiers	
CAS number	[78-93-3]
RTECS number	EL6475000
SMILES	CCC(=O)C
Properties	
Molecular formula	C ₄ H ₈ O CH ₃ COC ₂ H ₅
Molar mass	72.11 g/mol
Appearance	Colorless liquid
Density	0.8050 g/cm ³ , liquid
Melting point	−86 °C (187 K)
Boiling point	80 °C (353 K)
Solubility in water	29 g/100 ml (20 °C)

the ability to reproduce. Mice who breathed low levels for a short time showed temporary behavioral effects. Mild kidney damage was seen in animals that drank water with low levels of butanone for a short time.

There are no long-term studies with animals either breathing or drinking butanone.

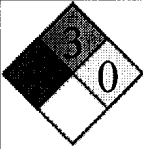
Methyl ethyl ketone is listed as a Table II precursor under the United Nations Convention Against Illicit Traffic in Narcotic Drugs and Psychotropic Substances[1].

References

External links

- International Chemical Safety Card 0179
 - National Pollutant Inventory - Methyl Ethyl Ketone Fact Sheet
 - NIOSH Pocket Guide to Chemical Hazards
 - US EPA Datasheet
-
- US NIH list of products that contain butanone (MEK)

Retrieved from "<http://en.wikipedia.org/wiki/Butanone>"
Categories: Ketones | Ketone solvents | DEA List II chemicals
Hidden categories: Articles lacking sources from October 2007 | All articles lacking sources

Viscosity	0,43 cP at 20 °C
Structure	
Dipole moment	2.76 D
Hazards	
MSDS	External MSDS
EU classification	Flammable (F) Irritant (Xi)
NFPA 704	
R-phrases	R11, R36, R66, R67
S-phrases	(S2), S9, S16
Flash point	−9 °C
Autoignition temperature	505 °C
Related compounds	
Related Ketones	Acetone; 3-pentanone; 3-Methylbutanone
Supplementary data page	
Structure and properties	<i>n</i> , <i>ε</i> _r , etc.
Thermodynamic data	Phase behaviour Solid, liquid, gas
Spectral data	UV, IR, NMR, MS
Except where noted otherwise, data are given for materials in their standard state (at 25 °C, 100 kPa) Infobox disclaimer and references	

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Toluene

From Wikipedia, the free encyclopedia

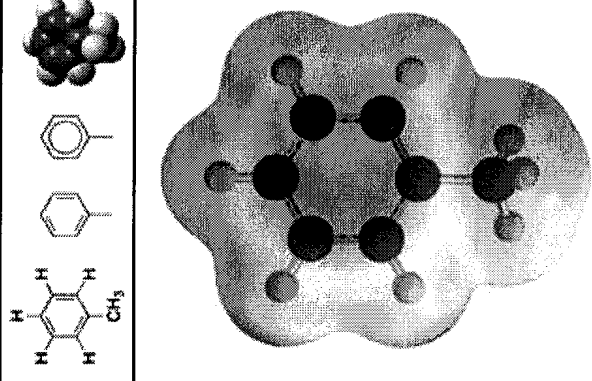
Toluene, also known as **methylbenzene** or **phenylmethane**, is a clear, water-insoluble liquid with the typical smell of paint thinners, redolent of the sweet smell of the related compound benzene. It is an aromatic hydrocarbon that is widely used as an industrial feedstock and as a solvent. Like other solvents, toluene is also used as an inhalant drug for its intoxicating properties.^{[1][2]}

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History

Toluene



The name *toluene* was derived from the older name *toluol*, which refers to tolu balsam, an aromatic extract from the tropical Colombian tree *Myroxylon balsamum*, from which it was first isolated. It was originally named by Jöns Jakob Berzelius.

Chemical properties

Toluene reacts as a normal aromatic hydrocarbon towards electrophilic aromatic substitution. [3][4]

[5] The methyl group makes it around 2.5 times more reactive than benzene in such reactions. It undergoes smooth sulfonation to give *p*-toluenesulfonic acid, and chlorination by Cl₂ in the presence of FeCl₃ to give ortho and para isomers of chlorotoluene. It undergoes nitration to give ortho and para nitrotoluene isomers, but if heated it can give dinitrotoluene and ultimately the explosive trinitrotoluene (TNT).

With other reagents the methyl side chain in toluene may react, undergoing oxidation. Reaction with potassium permanganate leads to benzoic acid, whereas reaction with chromyl chloride leads to benzaldehyde (Étard reaction). Halogenation can be performed under free radical conditions. For example, *N*-bromosuccinimide (NBS) heated with toluene in the presence of AIBN leads to benzyl bromide.

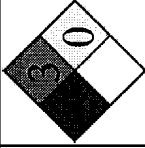
Catalytic hydrogenation of toluene to methylcyclohexane requires a high pressure of hydrogen to go to completion, because of the stability of the aromatic system. pKa is approximately 45.

Preparation

Toluene occurs naturally at low levels in crude oil and is usually produced in the processes of making gasoline via a catalytic reformer, in an ethylene cracker or making coke from coal. Final separation (either via distillation or solvent extraction) takes place in a BTX plant.

Uses

Toluene is a common solvent, able to dissolve: paints, paint thinners, silicone sealants, [6] many chemical reactants, rubber, printing ink, adhesives (glues), lacquers, leather tanners, and disinfectants. It can also be used as a fullerene indicator, and is a raw material for toluene diisocyanate (used in the manufacture of polyurethane foam) and TNT. Industrial uses of toluene include dealkylation to benzene and disproportionation to a mixture of benzene and xylene. When oxidized it yields benzaldehyde and benzoic acid, two important intermediates in chemistry. It is

Other names	phenylmethane toluol methylbenzene
Identifiers	
CAS number	[108-88-3]
RTECS number	XS5250000
SMILES	Cc1ccccc1
Properties	
Molecular formula	C ₇ H ₈ (C ₆ H ₅ CH ₃)
Molar mass	92.14 g/mol
Appearance	Clear colorless, liquid
Density	0.8669 g/mL, liquid
Melting point	−93 °C
Boiling point	110.6 °C
Solubility in water	0.053 g/100 mL (20-25°C)
Viscosity	0.590 cP at 20°C
Structure	
Dipole moment	0.36 D
Hazards	
MSDS	External MSDS
MSDS	ScienceLab.com
Main hazards	highly flammable
NFPA 704	
R-phrases	R11, R38, R48/20, R63, R65, R67
S-phrases	(S2), S36/37, S29, S46, S62
Flash point	4 °C/ 39.2 °F

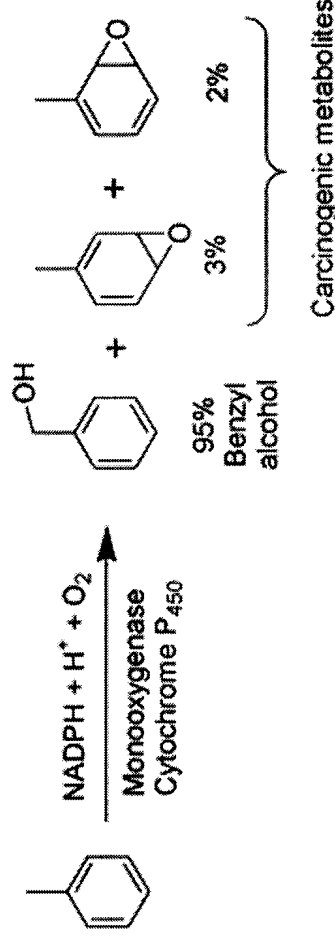
also used as a carbon source for making Multi-Wall Carbon Nanotubes. Toluene can be used to break open red blood cells in order to extract hemoglobin in biochemistry experiments.

Toluene can be used as an octane booster in gasoline fuels used in internal combustion engines. Toluene at 86% by volume, fueled all the turbo Formula 1 teams in the 1980s.

Toxicology and metabolism

Inhalation of toluene fumes can be intoxicating, but in larger doses nausea-inducing. Toluene may enter the human system not only through vapour inhalation from the liquid evaporation, but also following soil contamination events, where human contact with soil, ingestion of contaminated groundwater or soil vapour off-gassing can occur.

The toxicity of toluene can be explained mostly by its metabolism. As toluene has very low water solubility, it cannot exit the body via the normal routes (urine, feces, or sweat). It must be metabolized in order to be excreted. The methyl group of toluene is more easily oxidized by cytochrome P450 than the benzene ring. Therefore, in the metabolism of toluene, 95% is oxidized to become benzyl alcohol.^[7] The toxic metabolites are created by the remaining 5% that are oxidized to benzaldehyde and cresols.^{[8][9]} Most of the reactive products are detoxified by conjugation to glutathione but the remainder may severely damage cells.^[10]



Toluene is mainly excreted as benzoic acid and hippuric acid, both formed by further metabolic oxidation of benzyl alcohol.

Related compounds	
Related aromatic hydrocarbon	benzene xylene naphthalene
Related compounds	methylcyclohexane
Supplementary data page	
Structure and properties	n , ϵ_r , etc.
Thermodynamic data	Phase behaviour Solid, liquid, gas
Spectral data	UV, IR, NMR, MS
Except where noted otherwise, data are given for materials in their standard state (at 25 °C, 100 kPa) Infobox disclaimer and references	

Cyclohexanone

From Wikipedia, the free encyclopedia

Cyclohexanone is a six-carbon cyclic molecule with a ketone functional group. It is a colorless, oily liquid with an odor reminiscent of oil of peppermint and acetone. Over time, the color of the liquid changes to yellow. Cyclohexanone is slightly soluble in water (5-10 g/100 ml), but miscible with the most common organic solvents.

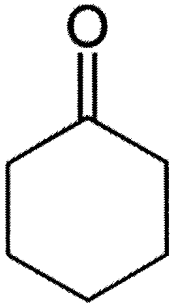

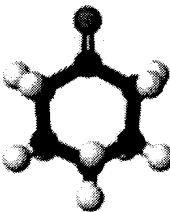
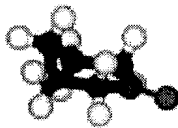
Cyclohexanone is employed as an industrial solvent and as activator in oxidation reactions. It is also used in the production of adipic acid, cyclohexanone resins, caprolactam and nylon 6.^[3]

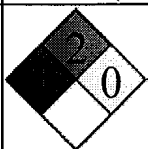
References

- ↑ International Chemical Safety Card 0425
- ↑ NIOSH Pocket Guide to Chemical Hazards
- ↑ Cyclohexanone at Chemicalland21.com

Retrieved from "http://en.wikipedia.org/wiki/Cyclohexanone"

Categories: Ketones | IARC Group 3 carcinogens

Cyclohexanone ^{[1][2]}	
	
	
Identifiers	
CAS number	[108-94-1]
SMILES	C1CCCCC1=O
Properties	
Molecular formula	C ₆ H ₁₀ O
Molar mass	98.15 g/mol
Appearance	Colorless, liquid
Density	0.9478 g/mL, liquid
Melting point	−16.4 °C
Boiling point	155.65 °C
Solubility in water	Slightly soluble
Solubility in ethanol	Miscible
Viscosity	0.898 cP at 25 °C
Thermochemistry	
Std enthalpy of formation Δ _f <i>H</i> [⦿] ₂₉₈	−270.7 kJ mol ^{−1}
Std enthalpy of	

combustion $\Delta_c H^\circ_{298}$	$-3519.3 \text{ kJ/mol}^{-1}$
Standard molar entropy S°_{298}	$+229.03 \text{ J.K}^{-1}.\text{mol}^{-1}$
Hazards	
EU classification	Harmful (Xn)
NFPA 704	
R-phrases	R10, R20
S-phrases	(S2), S25
Flash point	44 C
Related compounds	
Related ketones	Cyclopentanone
Related compounds	Cyclohexanol
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